LE MATEMATICHE
Vol. XLVIII (1993) – Fasc. I, pp. 109-122

THE CRF-METHOD FOR SEMICONDUCTORS' INTRAVALLEY COLLISION KERNELS: II - The 3D case

CLAUDIO BARONE - SANTO MOTTA

If the collisions are redefined as a flux a kinetic conservation law can be written in divergence form. This can be handled numerically, in the framework of Finite Particle Approximation, using the CRF-method. In this paper we use the CRF-method for the semiconductors' intravalley collision kernels. We extend the results obteined in a previous paper to the case of a 3D momentum space.

1. Introduction.

Semiconductors kinetic transport equation has been usually treated numerically using the Monte Carlo methods [5], [6]. For a few years Deterministic Particles Methods have been proposed as an alternative scheme for this class of problems [3], [4], [10], [11], [13]. In this framework the CRF-method for kinetic equations has been recently presented [2], [12]. The idea of the method is to write a conservation law in divergence form. This can be done easily by introducing a flux equivalent to the inhomogeneity. In a classical frame, the reciprocal of the desired function multiplied by the flux gives a velocity field. However, in the finite point approximation a reciprocal does not exist. Since the velocity field can also be interpreted as the Radon-Nikodym derivative of the flux, we use the latter for a numerical approximation. This gives a scheme where

Entrato in Redazione il 15 marzo 1993.

Key words and phrases: Kinetic equations, Semiconductors.

the numerical effort depends only on the desired accuracy and not directly on the dimension of the phase space. In a previous paper [1] we have derived the relevant quantities needed for the numerical scheme in a 2D momentum space for the intravalley semiconductors kernels. In this paper we present the same analysis in a 3D momentum space.
We assume that the energy-momentum relationship can be treated in the parabolic approximation. Under this assumption the natural coordinate system for the problem is the spherical one. Then one should use the CRF-method formulation in generalized coordinates [2]. As shown in [1] one can use the existing similarities between the semiconductors' intravalley collision kernels to identify three different model kernels. This will optimize the analytical work and reduce the implementation effort.

2. Semiconductors' intravalley model kernels.

In the semiclassical approach the collision term for semiconductors can be expressed as the difference between the electrons scattered in and out of the state k

$$(1) \quad Q(f) = \int_{\Omega} \left(S(k', k) f(k')(1 - f(k)) - S(k, k') f(k)(1 - f(k'))\right) dk'$$

where $S(k, k')$ represents the probability per unit time of an electron transition from a state k into an empty state k', induced by the lattice imperfections. The $(1 - f)$ coefficients accounts for the Pauli exclusion principle. In many case these factors do not contributes since it is always assumed $f \ll 1$ [6].

The transition probability $S(k, k')$ from the initial state k to the final state k', having energies ε and ε', due to a given interaction mechanisme, is given [6], [14]

$$S(k, k') = \frac{V_0}{(2\pi)^3} \frac{2\pi}{\hbar} ||V(k - k')||^2 G((k, k')\delta(\varepsilon' - \varepsilon)$$

where V_0 is the volume of the crystal, $G(k', k)$ is the overlap integral and $||V(k - k')||^2$ is the square of the matrix element of the interaction mechanism. For electrons intravalley transition process G is equal to unity [6].

In the previous paper [1] we have pointed out that most of the relevant intravalley interaction mechanism can be described – by suitably changing the meaning and the values of the constants – through three model kernels

$$(2) \qquad S(k, k') = A\delta(k'^2 - k^2 + \varphi)$$

$$S(k,k') = \frac{A}{||k-k'||^2}\delta(k'^2 - k^2 + \varphi) \tag{3}$$

$$S(k,k') = \frac{A}{(||k-k'||^2 + \beta^2)^2}\delta(k'^2 - k^2)\,. \tag{4}$$

Here we have used the parabolic approximation $\varepsilon = \hbar k^2/2m^*$. The constant φ is obviously suitably defined.
All the other relevant kernels can then be derived from these [4] and one can minimize both the analytical effort and the code writing.

As shown in section 2 of [1] the solution of the equation of motion reduces to the computation of the vector field g. We are the involved in computing the r.h.s. of the equation (15) of [1], i.e. the Ψ^i. Here we want to use spherical coordinates. For this purpose let (ξ_1, ξ_2, ξ_3), (k_1, k_2, k_3) respectively the Cartesian and the spherical coordinates, $\Omega_k = [\alpha_1, \beta_1] \times [0, \pi] \times [0, 2\pi]$, and denote by T the coordinate transformation from $\{\xi\} \to \{k\}$ and by $|T| = k_1^2 \sin k_2$ its Jacobian. The collision term for semiconductors can be expressed as the difference between a gain term G and a lost term L. Then in the new coordinate system we have

$$\widetilde{Q}(\widetilde{f}(k_1,k_2,k_3)) = \widetilde{G}(k_1,k_2,k_3) - \widetilde{L}(k_1,k_2,k_3)$$

where $\widetilde{G}$ and $\widetilde{L}$ are given by

$$\widetilde{G}(k_1,k_2,k_3) = \int_{\Omega_\mu} S(\mu_1,\mu_2,\mu_3,k_1,k_2,k_3)\widetilde{f}(\mu_1,\mu_2,\mu_3)k_1^2 \sin k_2\, d\mu \tag{5}$$

$$\widetilde{L}(k_1,k_2,k_3) = \widetilde{f}(k_1,k_2,k_3)\widetilde{C}(k_1,k_2,k_3) \tag{6}$$

with

$$\widetilde{C}(k_1,k_2,k_3) = \int_{\Omega_\mu} S(k_1,k_2,k_3,\mu_1,\mu_2,\mu_3)\mu_1^2 \sin \mu_2\, d\mu \tag{7}$$

where $\mu = (\mu_1, \mu_2, \mu_3)$. Then the $\Psi^i(\gamma_i)$ can be written in the form

$$\Psi^i(\gamma_i) = -\Psi^i_{\widetilde{G}}(\gamma_i) + \Psi^i_{\widetilde{L}}(\gamma_i). \tag{8}$$

To evaluate the $\Psi^i(\gamma_i)$ for $i = 1, 2, 3$ we can proceed as in [1]:

1. We approximate the density function $\widetilde{f}(t,k)$ by a discrete measure
$$\widetilde{f}(t,k_1,k_2,k_3) = f(t,k_1,k_2,k_3)\,|T| = \\ = \frac{1}{N}\sum_{j=1}^{N} \delta(k_1 - k_{1,j})\,\delta(k_2 - k_{2,j})\,\delta(k_3 - k_{3,j});$$
2. Compute $\widetilde{G}(k)$ and $\widetilde{L}(k)$;
3. Compute $\Psi^i(\gamma_i)$, $i = 1, 2, 3$, separately for $\widetilde{G}(k)$ and $\widetilde{L}(k)$.

After some algebra, variable transformations and appropriate use of the Heaviside function $H(\cdot)$ we get the following results.

1. MODEL KERNEL (2).

$$\widetilde{G}(k) = \frac{1}{N}\sum_{j=1}^{N} S(k_j, k) \tag{9}$$

$$\widetilde{C}(k) = 2\pi A\sqrt{k_1^2 - \varphi}\, H\left[(k_1^2 - \varphi - \alpha_1^2)(\beta_1^2 - k_1^2 + \varphi)\right]. \tag{10}$$

Then we compute the Ψ components. Setting $a_j = k_{1,j}^2 - \varphi$ for the first component we get

$$\Psi_{\widetilde{G}}^1(\gamma_1) = \frac{2\pi A}{N}\sum_{j=1}^{N}(\gamma_1 - \sqrt{a_j})\sqrt{a_j}H[(a_j - \alpha_1^2)(\gamma_1^2 - a_j)] \tag{11}$$

$$\Psi_{\widetilde{L}}^1(\gamma_1) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_1 - k_{1,j})\widetilde{C}(k_j)H(\gamma_1 - k_{1,j}). \tag{12}$$

For the second component we get

$$\Psi_{\widetilde{G}}^2(\gamma_2) = \frac{\pi A(\gamma_2 - \sin\gamma_2)}{N}\sum_{j=1}^{N}\sqrt{a_j}H\left[(a_j - \alpha_1^2)(\beta_1^2 - a_j)\right] \tag{13}$$

$$\Psi_{\widetilde{L}}^2(\gamma_2) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_2 - k_{2,j})\widetilde{C}(k_j)H(\gamma_2 - k_{2,j}). \tag{14}$$

For the third component we get

$$\Psi_{\widetilde{G}}^3(\gamma_3) = \frac{A\gamma_3^2}{2N}\sum_{j=1}^{N}\sqrt{a_j}H\left[(a_j - \alpha_1^2)(\beta_1^2 - a_j)\right] \tag{15}$$

$$\Psi_{\widetilde{L}}^3(\gamma_3) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_3 - k_{3,j})\widetilde{C}(k_j)H(\gamma_3 - k_{3,j}). \tag{16}$$

We note that in the elastic limit we get $\Psi_{\widetilde{G}}^1(\gamma_1) = \Psi_{\widetilde{L}}^1(\gamma_1)$ as required.

2. MODEL KERNEL (3).

$$\widetilde{G}(k) = \frac{1}{N}\sum_{j=1}^{N}\widetilde{S}(k_j, k) \tag{17}$$

$$\widetilde{C}(k) = \frac{A}{2}\sqrt{k_1^2 - \varphi}F(k)H\left[(k_1^2 - \varphi - \alpha_1^2)(\beta_1^2 - k_1^2 + \varphi)\right] \tag{18}$$

where

(19) $F(k) =$

$$= \int_0^{\pi}\int_0^{2\pi} \frac{\sin k_2'\, dk_2' dk_3'}{2k_1^2 - \varphi - 2k_1\sqrt{k_1^2 - \varphi}\left[\sin k_2 \sin k_2' \cos(k_3 - k_3') + \cos k_2 \cos k_2'\right]}.$$

Then we compute the Ψ components. Setting $a_j = k_{1,j}^2 - \varphi$ for the first component we get

$$\Psi_{\widetilde{G}}^1(\gamma_1) = \frac{A}{2N}\sum_{j=1}^{N}(\gamma_1 - \sqrt{a_j})\sqrt{a_j}F_1(\sqrt{a_j}, k_j)H\left[(a_j - \alpha_1^2)(\gamma_1^2 - a_j)\right] \tag{20}$$

$$\Psi_{\widetilde{L}}^1(\gamma_1) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_1 - k_{1,j})\widetilde{C}(k_j)H(\gamma_1 - k_{1,j}) \tag{21}$$

where

(22) $F_1(k_1', k_j) =$

$$= \int_0^{\pi}\int_0^{2\pi} \frac{\sin k_2\, dk_2 dk_3}{k_{1,j}^2 + k_1'^2 - 2k_{1,j}k_1'\left[\sin k_{2,j} \sin k_2 \cos(k_{3,j} - k_3) + \cos k_{2,j} \cos k_2\right]}$$

For the second component we get

$$\Psi_{\widetilde{G}}^2(\gamma_2) = \frac{A}{2N}\sum_{j=1}^{N}\sqrt{a_j}H\left[(a_j - \alpha_1^2)(\beta_1^2 - a_j)\right]\int_0^{\gamma_2} F_2(k_2, k_j)\, dk_2 \tag{23}$$

$$\Psi_{\widetilde{L}}^2(\gamma_2) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_2 - k_{2,j})\widetilde{C}(k_j)H(\gamma_2 - k_{2,j}) \tag{24}$$

where

(25) $$F_2(k_2, k_j) = = \int_0^{2\pi}\int_0^{k_2} \frac{\sin k_2'\, dk_2' dk_3}{k_{1,j}^2 + a_j - 2k_{1,j}\sqrt{a_j}\left[\sin k_{2,j} \sin k_2' \cos(k_{3,j} - k_3) + \cos k_{2,j} \cos k_2'\right]}$$

For the third component we get

(26) $$\Psi_{\widetilde{G}}^3(\gamma_3) = \frac{A}{2N}\sum_{j=1}^{N} \sqrt{a_j} H\left[(a_j - \alpha_1^2)(\beta_1^2 - a_j)\right] \int_0^{\gamma_3} F_3(k_3, k_j)\, dk_3$$

(27) $$\Psi_{\widetilde{L}}^3(\gamma_3) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_3 - k_{3,j})\widetilde{C}(k_j) H(\gamma_3 - k_{3,j})$$

where

(28) $$F_3(k_3, k_j) = = \int_0^{\pi}\int_0^{k_3} \frac{\sin k_2\, dk_2 dk_3'}{k_{1,j}^2 + a_j - 2k_{1,j}\sqrt{a_j}\left[\sin k_{2,j} \sin k_2 \cos(k_{3,j} - k_3') + \cos k_{2,j} \cos k_2\right]}$$

The calculation of the integral functions defined by equations (22), (25) and g is presented in appendix A, while the r.h.s. integrals in (23) and (26) must be computed numerically.
Furthermore we note that in the elastic limit we get $\Psi_{\widetilde{G}}^1(\gamma_1) = \Psi_{\widetilde{L}}^1(\gamma_1)$ as required.

3. MODEL KERNEL (4).

(29) $$\widetilde{G}(k) = \frac{1}{N}\sum_{j=1}^{N} \widetilde{S}(k_j, k)$$

(30) $$\widetilde{C}(k) = \frac{A}{2} k_1 F(k) H\left[(k_1^2 - \alpha_1^2)(\beta_1^2 - k_1^2)\right]$$

where

(31) $$F(k) = = \int_0^{\pi}\int_0^{2\pi} \frac{\sin k_2'\, dk_2' dk_3'}{\left[2k_1^2 - 2k_1^2(\sin k_2 \sin k_2' \cos(k_3 - k_3') + \cos k_2 \cos k_2') + \beta^2\right]^2}.$$

Then we compute the Ψ components. For the first component we get

$$\Psi^1_{\tilde{G}}(\gamma_1) = \frac{A}{2N}\sum_{j=1}^{N} k_{1,j}(\gamma_1 - k_{1,j})F_1(k_{1,j}, k_j)H(\gamma_1^2 - k_{1,j}) \tag{32}$$

$$\Psi^1_{\tilde{L}}(\gamma_1) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_1 - k_{1,j})\widetilde{C}(k_j)H(\gamma_1 - k_{1,j}) \tag{33}$$

where

$$F_1(k_1', k_j) = \tag{34}$$
$$= \int_0^{\pi}\int_0^{2\pi} \frac{\sin k_2\, dk_2 dk_3}{\left[\alpha - 2k_{1,j}k_1'(\sin k_{2,j}\sin k_2 \cos(k_{3,j} - k_3) + \cos k_{2,j}\cos k_2)\right]^2}$$

with $\alpha = k_{1,j}^2 + k_1'^2 + \beta^2$.
For the second component we get

$$\Psi^2_{\tilde{G}}(\gamma_2) = \frac{A}{2N}\sum_{j=1}^{N} k_{1,j}\int_0^{\gamma_2} F_2(k_2, k_j)\, dk_2 \tag{35}$$

$$\Psi^2_{\tilde{L}}(\gamma_2) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_2 - k_{2,j})\widetilde{C}(k_j)H(\gamma_2 - k_{2,j}) \tag{36}$$

where

$$F_2(k_2, k_j) = \tag{37}$$
$$= \int_0^{2\pi}\int_0^{k_2} \frac{\sin k_2'\, dk_2' dk_3}{\left[2k_{1,j}^2 - 2k_{1,j}^2(\sin k_{2,j}\sin k_2' \cos(k_{3,j} - k_3) + \cos k_{2,j}\cos k_2') + \beta^2\right]^2}$$

For the third component we get

$$\Psi^3_{\tilde{G}}(\gamma_3) = \frac{A}{2N}\sum_{j=1}^{N} k_{1,j}\int_0^{\gamma_3} F_3(k_3, k_j)\, dk_3 \tag{38}$$

$$\Psi_L^3(\gamma_3) = \frac{1}{N}\sum_{j=1}^{N}(\gamma_3 - k_{3,j})\widetilde{C}(k_j)H(\gamma_3 - k_{3,j}) \tag{39}$$

where

$$F_3(k_3, k_j) = \tag{40}$$
$$= \int_0^\pi \int_0^{k_3} \frac{\sin k_2\, dk_2 dk_3'}{\left[2k_{1,j}^2 - 2k_{1,j}^2(\sin k_{2,j}\sin k_2 \cos(k_{3,j} - k_3') + \cos k_{2,j}\cos k_2) + \beta^2\right]^2}$$

The calculation of the integral functions defined by equations (34), (37) and (40) is presented in appendix A, while the r.h.s. integrals in (35) and (38) must be computed numerically.
This model kernel is already elastic. This Property is conserved by the CRF-method as can be seen, with simple algebra, from (32) and (33).

3. Conclusions.

The numerical experiments performed using the CRF-method, performed for a 2D model using the Polar Optical Scattering collision kernel, show that the method can be used for numerical computations [2]. For this we have computed the relevant quantities for the application of the method to intravalley model kernels in a 3D momentum space.

Acknowledgments. This work has been partially supported by CRN (grant n. 91.02198.CT11 – Comitato Naz. Ric. Tecnologiche ed Innovazione; grant n. 91.00911.69 – Progetto Finalizzato Calcolo Parallelo) and M.U.R.S.T.

Appendix A.

In this appendix we compute the integral functions defined by equations (22), (25), (28), (34), (37) and (28).

We consider first the integral functions (22), (25), (28). These can be written in the following equivalent ways

$$\begin{aligned} F_1(k_1', k_j) &= \int_0^\pi \overline{F}_1(k_1', k_2, k_j)\sin k_2\, dk_2 \\ &= \int_0^{2\pi} \widetilde{F}_1(k_1', k_3, k_j)\, dk_3 \end{aligned} \tag{41}$$

$$
\begin{aligned}
F_2(k_2, k_j) &= \int_0^{k_2} \overline{F}_2(k_2', k_j) \sin k_2' \, dk_2' \\
&= \int_0^{2\pi} \widetilde{F}_2(k_2, k_3, k_j) \, dk_3
\end{aligned} \tag{42}
$$

$$
\begin{aligned}
F_3(k_3, k_j) &= \int_0^{k_3} \widetilde{F}_3(k_3', k_j) \, dk_3 \\
&= \int_0^{\pi} \overline{F}_3(k_2, k_3, k_j) \sin k_2 \, dk_2
\end{aligned} \tag{43}
$$

where

$$\overline{F}_1(k_1', k_2, k_j) = \int_0^{2\pi} \frac{dk_3}{\overline{a}_1 - \overline{b}_1 \cos(k_{3,j} - k_3)} \tag{44}$$

$$\widetilde{F}_1(k_1', k_3, k_j) = \int_0^{\pi} \frac{\sin k_2}{\widetilde{a}_1 + \widetilde{b}_1 \sin k_2 + \widetilde{c}_1 \cos k_2} \, dk_2 \tag{45}$$

$$\overline{F}_2(k_2', k_j) = \int_0^{2\pi} \frac{dk_3}{\overline{a}_2 - \overline{b}_2 \cos(k_{3,j} - k_3)} \tag{46}$$

$$\widetilde{F}_2(k_2, k_3, k_j) = \int_0^{k_2} \frac{\sin k_2'}{\widetilde{a}_2 + \widetilde{b}_2 \sin k_2' + \widetilde{c}_2 \cos k_2'} \, dk_2' \tag{47}$$

$$\widetilde{F}_3(k_3', k_j) dk_3 = \int_0^{\pi} \frac{\sin k_2}{\widetilde{a}_3 + \widetilde{b}_3 \sin k_2 + \widetilde{c}_3 \cos k_2} \, dk_2 \tag{48}$$

$$\overline{F}_3(k_2, k_3, k_j) = \int_0^{k_3} \frac{dk_3'}{\overline{a}_3 - \overline{b}_3 \cos(k_{3,j} - k_3')} \tag{49}$$

with

$$
\begin{aligned}
\overline{a}_1 &= k_{1,j}^2 + k_1' - 2k_{1,j} k_1' \cos k_{2,j} \cos k_2 \\
\overline{b}_1 &= 2k_{1,j} k_1' \sin k_{2,j} \sin k_2 \\
\overline{a}_2 &= k_{1,j}^2 + a_j - 2k_{1,j} \sqrt{a_j} \cos k_{2,j} \cos k_2' \\
\overline{b}_2 &= 2k_{1,j} \sqrt{a_j} \sin k_{2,j} \sin k_2' \\
\overline{a}_3 &= k_{1,j}^2 + a_j - 2k_{1,j} \sqrt{a_j} \cos k_{2,j} \cos k_2 \\
\overline{b}_3 &= 2k_{1,j} \sqrt{a_j} \sin k_{2,j} \sin k_2
\end{aligned}
$$

and

$$
\begin{aligned}
\widetilde{a}_1 &= k_{1,j}^2 + k_1' \\
\widetilde{b}_1 &= -2k_{1,j}k_1' \sin k_{2,j} \cos(k_{3,j} - k_3) \\
\widetilde{c}_1 &= -2k_{1,j}k_1' \cos k_{2,j} \\
\widetilde{a}_2 &= k_{1,j}^2 + a_j \\
\widetilde{b}_2 &= -2k_{1,j}\sqrt{a_j} \sin k_{2,j} \cos(k_{3,j} - k_3) \\
\widetilde{c}_2 &= -2k_{1,j}\sqrt{a_j} \cos k_{2,j} \\
\widetilde{a}_3 &= k_{1,j}^2 + a_j \\
\widetilde{b}_3 &= -2k_{1,j}\sqrt{a_j} \sin k_{2,j} \cos(k_{3,j} - k_3') \\
\widetilde{c}_3 &= -2k_{1,j}\sqrt{a_j} \cos k_{2,j}\,.
\end{aligned}
$$

We note that the integral functions defined by equations (44), (45), (46), (47), (48) and (49) can be computed analytically (see appendix B and appendix A of [1]), while the integrals on the r.h.s. of the equations (41), (42) and (43) must be computed numerically. Moreover, as pointed out, there are two equivalent ways to compute the integral functions F_1, F_2 and F_3. The choice of the most convenient way needs to be carefully evaluted.

We now consider the integral functions (34), (37), (40). These can also be written in the forms (41), (42) and (43) respectively, where

$$\overline{F}_1(k_1', k_2, k_j) = \int_0^{2\pi} \frac{dk_3}{\left[\overline{a}_1 - \overline{b}_1 \cos(k_{3,j} - k_3)\right]^2} \tag{50}$$

$$\widetilde{F}_1(k_1', k_3, k_j) = \int_0^{\pi} \frac{\sin k_2}{[\widetilde{a}_1 + \widetilde{b}_1 \sin k_2 + \widetilde{c}_1 \cos k_2]^2}\, dk_2 \tag{51}$$

$$\overline{F}_2(k_2', k_j) = \int_0^{2\pi} \frac{dk_3}{[\overline{a}_2 - \overline{b}_2 \cos(k_{3,j} - k_3)]^2} \tag{52}$$

$$\widetilde{F}_2(k_2, k_3, k_j) = \int_0^{k_2} \frac{\sin k_2'}{[\widetilde{a}_2 + \widetilde{b}_2 \sin k_2' + \widetilde{c}_2 \cos k_2']^2}\, dk_2' \tag{53}$$

$$\widetilde{F}_3(k_3', k_j) dk_3 = \int_0^{\pi} \frac{\sin k_2}{[\widetilde{a}_3 + \widetilde{b}_3 \sin k_2 + \widetilde{c}_3 \cos k_2]^2}\, dk_2 \tag{54}$$

$$\overline{F}_3(k_2, k_3, k_j) = \int_0^{k_3} \frac{dk_3'}{[\overline{a}_3 - \overline{b}_3 \cos(k_{3,j} - k_3')]^2} \tag{55}$$

with

$$\begin{aligned}
\overline{a}_1 &= k_{1,j}^2 + k_1'^2 + \beta^2 - 2k_{1,j}k_1' \cos k_{2,j} \cos k_2 \\
\overline{b}_1 &= 2k_{1,j}k_1' \sin k_{2,j} \sin k_2 \\
\overline{a}_2 &= 2k_{1,j}^2 + \beta^2 - 2k_{1,j}^2 \cos k_{2,j} \cos k_2' \\
\overline{b}_2 &= 2k_{1,j}^2 \sin k_{2,j} \sin k_2' \\
\overline{a}_3 &= 2k_{1,j}^2 + \beta^2 - 2k_{1,j}^2 \cos k_{2,j} \cos k_2 \\
\overline{b}_3 &= 2k_{1,j}^2 \sin k_{2,j} \sin k_2
\end{aligned}$$

and

$$\begin{aligned}
\widetilde{a}_1 &= k_{1,j}^2 + k_1'^2 + \beta^2 \\
\widetilde{b}_1 &= -2k_{1,j}k_1' \sin k_{2,j} \cos(k_{3,j} - k_3) \\
\widetilde{c}_1 &= -2k_{1,j}k_1' \cos k_{2,j} \\
\widetilde{a}_2 &= 2k_{1,j}^2 + \beta^2 \\
\widetilde{b}_2 &= -2k_{1,j}^2 \sin k_{2,j} \cos(k_{3,j} - k_3) \\
\widetilde{c}_2 &= -2k_{1,j}^2 \cos k_{2,j} \\
\widetilde{a}_3 &= 2k_{1,j}^2 + \beta^2 \\
\widetilde{b}_3 &= -2k_{1,j}^2 \sin k_{2,j} \cos(k_{3,j} - k_3') \\
\widetilde{c}_3 &= -2k_{1,j}^2 \cos k_{2,j} \,.
\end{aligned}$$

Also in this case the integral functions defined by equations (50), (51), (52), (53), (54) and (55) can be computed analytically (see appendix B and appendix A of [1]), while the integrals on the r.h.s. of the equations (41), (42) and (43) must be computed numerically. Again the choice of the most convenient way to perform the integration needs to be carefully evaluated.

Appendix B.

In this appendix we recall the results of two well known generalized integrals which we have used in the previous calculations.

We consider first the integral

$$I(x) = \int \frac{\sin x}{a + b \sin x + c \cos x} dx \tag{56}$$

where a, b, c are real constants with $a^2 > b^2 + c^2$ and $a \neq c$. The primitive $I(x)$ can be computed analytically. Let

$$p = \frac{2b}{a-c}$$

$$q = \frac{a+c}{a-c}$$

$$t = \tan\frac{x}{2}\,.$$

Then we get

$$I(x) = \frac{4}{a-c}\int \frac{t}{(1+t^2)(t^2+pt+q)}\,dt\,. \tag{57}$$

The r.h.s. integral of the equation (57) can be split in the following way

$$\int \frac{t}{(1+t^2)(t^2+pt+q)}\,dt = \int \frac{At+B}{1+t^2}\,dt + \int \frac{Ct+D}{t^2+pt+q}\,dt \tag{58}$$

where A, B, C, D are the following constants

$$A = \frac{q-1}{p^2+(q-1)^2}$$

$$B = \frac{p}{p^2+(q-1)^2}$$

$$C = -A$$

$$D = -qB.$$

The integrals on the r.h.s. of the equation (58) can be easily calculated and we have

$$\int \frac{At+B}{1+t^2}\,dt = \frac{A}{2}\log(1+t^2) + B\arctan t$$

$$\int \frac{Ct+D}{t^2+pt+q}\,dt = \frac{C}{2}\log(t^2+pt+q) + \left(D - \frac{pC}{2}\right)\frac{2}{\sqrt{4q-p^2}}\arctan\frac{2t+p}{\sqrt{4q-p^2}}\,.$$

We note that, if $\pi \in [\alpha, \beta]$, we have

$$\int_{\alpha}^{\beta} \frac{\sin x}{a + b \sin x + c \cos x} dx = I(\pi^{-}) - I(\alpha) + I(\beta) - I(\pi^{+}).$$

We now consider the integral

$$J(x) = \int \frac{\sin x}{(a + b \sin x + c \cos x)^2} dx \tag{59}$$

where a, b, c are real constants with $a^2 > b^2 + c^2$ and $a \neq c$. Again the primitive can be obtained in a closed form

$$\begin{aligned} J(x) = &-\frac{1}{2(a-c)(t^2 + pt + q)} - \\ &- \frac{8p\sqrt{4q - p^2}}{2(a-c)(4q - p^2)} \left\{ \frac{1}{2} \arctan y + \frac{y}{2(1 + y^2)} \right\}. \end{aligned} \tag{60}$$

where

$$p = \frac{2b}{a - c}$$

$$q = \frac{a + c}{a - c}$$

$$t = \tan \frac{x}{2}$$

$$y = 2t + p\sqrt{4q - p^2}.$$

Also in this case, if $\pi \in [\alpha, \beta]$, we have

$$\int_{\alpha}^{\beta} \frac{\sin x}{(a + b \sin x + c \cos x)^2} dx = J(\pi^{-}) - J(\alpha) + J(\beta) - J(\pi^{+}).$$

REFERENCES

[1] C. Barone - S. Motta, *The CRF-method for Semiconductors' Intravalley Collision Kernels : I - The 2D case,* Le Matematiche, 47 (1992), pp. 163-175.

[2] R. Burkhard - S. Motta - J. Wick, *The CRF-method in general coordinates,* preprint, 1992.

[3] P. Degond - F. Guyot-Delaurens - F.J. Mustieles - F. Nier, *Simulation Particulaire du trasport bidimensionnel d'electrons parallele a l'interface d'une heterojonction,* rapport interne n.189, Ecole Polytechnique, Palaiseau, 1989.

[4] P. Degond - F.J. Mustieles, *Le Logicien SPADES-1 Version 2,* Documentation Scientifique, Centre de Mathematiques Appliquees, Ecole Polytechnique, Palaiseau, 1990.

[5] R.W. Hockney - J.W. Eastwood, *Computer simulation Using Particles,* Adam Hilger, Bristol, 1988.

[6] C. Jacoboni - P. Lugli, *The MonteCarlo Method for Semiconductor Device simulation,* SpringerVerlag, Berlin, 1989.

[7] L.D. Landau - E.M. Lifshitz, *Quantum Mechanics,* Pergamon Press, 1964.

[8] A. Messiah, *Mecanique Quantique,* Dunod, Paris, 1965.

[9] P.M. Morse - H. Feshbach, *Methods of Theoretical Physics,* McGraw-Hill, New-York, 1953.

[10] S. Motta - G. Russo - H. Moock - J. Wick, *A Number-theoretical Convergence Proof of a Point Approximation of a Space Homogeneous Transport Equation,* Le Matematiche, 41 (1986), pp. 161-178.

[11] S. Motta - G. Russo - H. Moock - J. Wick, *Point Approximation of a Space Homogeneous Transport Equation,* Numer. Math., 56 (1990), pp. 763-774.

[12] S. Motta - J. Wick, *A New Numerical Method for Kinetic Equations in Several Dimensions,* Computing, 46 (1991), pp. 223-232.

[13] B. Niclot - P. Degond - F. Poupaud, *Deterministic Particle Simulation of the Boltzmann transport equation of semiconductors,* J. Comp. Phys., 78 (1988), pp. 313-349.

[14] L. Reggiani (Ed.), *Hot-Electron Transport in Semiconductors,* Springer Verlag, Berlin, 1985.

Dipartimento di Matematica,
Università di Catania,
Viale A. Doria 6,
95125 Catania (Italy)